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<p>(54) Title: UV ABSORBENT COMPOSITIONS</p>		
<p>(57) Abstract</p> <p>The invention relates to sun screen compositions comprising <u>octyl triazone</u> as ultra violet light absorber and at least one compound selected from the group consisting of iso-stearic acid and iso-stearyl alcohol. The latter two compounds may ensure a shift in the wavelength at which maximum absorbance occurs of octyl triazone.</p> <p style="text-align: center;">102(c)</p> <p style="text-align: center;">7-11,14</p> <p style="text-align: center;">103 12,15 13,16</p>		

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UV ABSORBENT COMPOSITIONS

The present invention relates to sun screen formulations comprising octyl triazone and a compound selected from the group consisting of iso-stearic acid and iso-stearyl alcohol.

5 The ultra violet light which reaches the earth causes coloration, decoloration, reduced strength, destruction etcetera of rubber, paints, ink, plastics etcetera leading to degradation of their quality. In order to prevent such degradation due to the ultra violet light, an ultra violet light absorbent(s) is added to products which contain such rubber, paint, ink, plastics etcetera.

10 Also, the ultra violet light causes acute skin reactions such as erythema and darkening, and may in the long term cause skin ageing and/or cancer. Due to this, sun screen cosmetics containing ultra violet light absorbents and/or ultra violet light scattering agents to address misgivings about the ill effect of the ultra violet light on the skin have been developed and a wide range of products have been introduced on the market.

15 Ultra violet light absorbing compounds (UV-absorbers) do not absorb the complete spectrum of ultra violet light to the same extent at each wavelength. Characteristics of UV-absorbers are therefore the wavelength at which absorption is largest (in nm), and the absorption percentage at this wavelength (relative, calculated using the law of Lambert-Beer). Both this wavelength and absorption percentage at maximum absorbency can be influenced by other components present together with the
20 UV-absorber.

The wavelength at which maximum absorbency occurs is an important factor in developing a sun screen formulation. For sun screens to be effective, it is generally preferred that the sun screen has a maximum absorbency at the wavelength causing the most extensive damage to the substrate or material concerned. For human skin, for
25 example, UV-B-light having a wavelength of about 307-308 nm is generally considered as being most damaging.

One of the known ultraviolet light (UV-light) absorbing compounds is octyl triazone. This compound is marketed under the trade name Uvinul T 150 by BASF. This compound has a maximum absorbency at approx. 312 nm, when measured in ethanol.

For many purposes, however, it can be desired that a sun screen formulation is used showing maximum absorbency at a different wavelength than 312 nm. For some purposes a higher wavelength can be desired, for other purposes a lower value, depending e.g. upon the substrate to which the sun screen formulation is to be applied. Therefore, it is an object of the present invention to provide a sun screen formulation comprising octyl triazone, having a maximum absorbency-wavelength at a different value than octyl triazone usually has, which is approximately 312 nm. Such a sun screen formulation should still have an acceptable absorption percentage (i.e. high enough). Furthermore, such a sun screen formulation preferably should not contain skin irritants. Moreover, it is desired that such compositions provide a further beneficial effect to the substrate to which it is applied (e.g. moisturizing effect in the case of application to the skin).

It has now been found that the above can be achieved by a UV-B-absorbing formulation or sun screen composition, comprising octyl triazone and at least one compound selected from the group consisting of iso-stearic acid, iso-stearyl alcohol, and mixtures thereof.

The terms 'UV-absorbing formulation', 'UV-absorbing composition', 'sun screen formulation' and 'sun screen composition' are used in the present application as synonymous terms. In the art 'sun screen formulations or compositions' are sometimes used in a more restrictive sense, i.e. as formulations and compositions which absorb UV light and which are intended for use on human skin and hair; this use is of particular interest in the present application.

It has been found that iso-stearic acid is capable of causing a hypsochromic shift of the wavelength for maximum absorbency (i.e. to shorter wavelength) of octyl triazone. Likewise, it has been found that iso-stearyl alcohol is capable of causing a

bathochromic shift of this wavelength (i.e. to longer wavelength) of octyl triazone.

Iso-stearic acid is herein to be understood as a saturated, branched fatty acid. The chain is predominantly methyl-branched. Such a product is e.g. known as the trade product PRISORINE 3505, of Unichema International, Gouda, the Netherlands. Iso-stearyl

5 alcohol is herein to be understood as a saturated, branched fatty alcohol. The chain is predominantly methyl-branched. Such a product is e.g. known as the trade product PRISORINE 3515, of Unichema International, Gouda, the Netherlands. Iso-stearyl alcohol can advantageously be prepared by reduction of iso-stearic acid. Both compounds have 18 carbon atoms.

10 When the sun screen formulations according to the invention are used for application to the skin of human beings, the use of iso-stearic acid and iso-stearyl alcohol has the advantage that such compounds are well acceptable to the skin (in the concentrations they are used). Moreover, these compounds are reported to be emollients. Additionally, the use of iso-stearic acid and iso-stearyl alcohol in conjunction with octyl
15 triazone has the additional advantage that maximum absorbance is still at an acceptable level.

In order to be effective, it is generally preferred that the sun screen formulation according to the invention comprises at least 0.5% by weight of octyl triazone. For some applications even higher levels of octyl triazone are desired, e.g. at least 1.5% by
20 weight of octyl triazone, or even at least 2.5% by weight, based on the final formulation.

The sun screen formulations according to the present invention preferably may contain up to 15% by weight of octyl triazone, based on the final formulation and more preferably up to 5% by weight. Consequently preferred amounts of octyl triazone are
25 0.5-15% by weight and more preferably 1.5-5% by weight, based on the final formulation.

The amount of iso-stearyl alcohol and/or iso-stearic acid in the sun screen formulations according to the present invention is at least 1% by weight, preferably at least 2% by

weight and most preferably at least 5% by weight, based on the final formulation. Preferably these formulations may contain up to 55% by weight, more preferably up to 40% by weight and most preferably up to 25% by weight of iso-stearyl alcohol and/or iso-stearic acid, based on the final formulation. Consequently preferred amounts are

5 1-55% by weight, more preferably 2-40% by weight and most preferably 5-25% by weight, based on the final formulation.

Iso-stearic acid and iso-stearyl alcohol can be used independently of each other in combination with octyl triazone. It can be preferred, however, depending upon the wavelength desired at which absorption should be largest, as well as on the maximum

10 absorbance desired, as well as on other properties like minimum amount of iso-stearic acid present, to use iso-stearic acid and iso-stearyl alcohol together with octyl triazone to provide a sun screen formulation. It has been found that good properties can be obtained when the compositions according to the invention comprise iso-stearic acid and iso-stearyl alcohol in a ratio of between 1:0.5 and 1:4. When a wavelength is

15 desired of around 308 nm at which absorption is largest, it is preferred that said ratio is between 1:1 and 1:3, depending upon the further constituents. Even more preferred is a ratio of between 1:1.5 and 1:2.5.

Octyl triazone, iso-stearic acid and iso-stearyl alcohol can be part of an oily formulation. For application on or in rubber, paints, plastics etcetera this is generally

20 the form which is most applicable.

Although such an oily formulation can be used on skin and hair of e.g. human beings, it is generally preferred to use sun screen formulations according to the invention which are in the form of oil and water emulsions. Such oily formulations and oil and water emulsions are made by methods known in the art. Oily formulations are made by

25 combining the ingredients and mixing them at elevated temperatures, usually between 50°C and 90°C. Oil and water emulsions are made by combining an oily formulation with water, optionally containing low amounts of additives like preservatives and humectants, and mixing them at elevated temperatures, usually between 50°C and 90°C; the oily formulation preferably contains a low amount of emulsifiers when used to

make such oil and water emulsions.

The formulations according to the present invention may contain, in addition to the octyl triazone and the iso-stearyl alcohol and/or iso-stearic acid, ingredients and additives which are conventionally employed in such UV-absorbing formulations or sun
5 screen formulations. Such ingredients include other emollients than iso-stearyl alcohol and/or iso-stearic acid, in particular those of animal or vegetable origin and more in particular those of vegetable origin, other UV-light absorbing compounds than octyl triazone; humectants; preservatives; emulsifiers; stabilisers; salts; perfumes and fragrances, like fragrance oils; moisturising agents; vitamins, like vitamin E and water.
10 The amount of the totality of these conventionally used ingredients preferably ranges from 30 to 98.5% by weight, based on the final formulation and most preferably from 70 to 93.5% by weight.

Although the present invention is mainly concerned with compositions comprising octyl triazone, the invention is also meant to encompass compositions containing a
15 simple derivative of octyl triazone in combination with at least one compound selected from the group consisting of iso-stearic acid and iso-stearyl alcohol, provided that similar effects of batho- and/or hypsochromic shift occur. Such simple derivatives can be octyl triazones containing simple substituents, which do not disrupt the electron delocalisation in the molecule. Such a substituent may be an alkoxy group preferably
20 having 6-22 carbon atoms or a dialkyl amino group wherein each alkyl group has preferably 1-6 carbon atoms. Preferably octyl triazone is used.

The present invention also encompasses the use of a compound selected from the group consisting of iso-stearic acid and iso-stearyl alcohol to cause a hypsochromic or bathochromic shift of octyl triazone in a sun screen composition. Said use should
25 preferably be within the boundaries and preferred ranges as set out above.

The invention is further illustrated by the following examples, which are not to be interpreted as limiting the invention thereto.

Example 1

The following solutions have been prepared:

- a. 50 ppm octyl triazone in ethanol
- b. 50 ppm octyl triazone in iso-stearic acid
- 5 c. 50 ppm octyl triazone in iso-stearyl alcohol

The octyl triazone used was Uvinul T 150, as marketed by BASF

The iso-stearic acid used was PRISORINE 3505 as marketed by Unichema International, the Netherlands.

The iso-stearyl alcohol used was PRISORINE 3515 as marketed by Unichema
10 International, the Netherlands.

Concentrations were chosen such as to avoid absorption higher than 1. The above three solutions a-c have been subjected to UV-absorbance measurements using a PE Lambda 2 UV-Spectrophotometer (Perkin Elmer), using a 1 mm cuvette.

The spectrophotometer was programmed with a scan between 290 nm and 400 nm. The
15 absorbance maximum (y-axis) was set to 1,000 to be within the Lambert-Beer law.

Iso-stearic acid and iso-stearyl alcohol have been subjected separately as well to check their own absorbance (1 mm cuvette). Both did not have any absorbance at any of the wavelengths measured.

Results are in table 1.

20 Table 1: 50 ppm octyl triazone in different media

Sample	Medium	Wavelength (nm) at max. abs.	Max. abs.
A	ethanol	311.9	0.584
B	iso-stearic acid	301.4	0.527
C	iso-stearyl alcohol	314.4	0.636

This example shows the bathochromic and hypsochromic shift of iso-stearyl alcohol and iso-stearic acid, respectively.

Example 2

Solutions have been prepared of 50 ppm octyl triazone in mixtures of iso-stearic acid and iso-stearyl alcohol, in mixture ratios of between 1:5 and 5:1. Of these solutions, the wavelength at maximum absorbency was measured in the same way as in example 1. Results are in table 2.

Table 2: 50 ppm octyl triazone in mixtures of iso-stearic acid/iso-stearyl alcohol

Sample	Wave length at max. abs. (nm)
1:5	310.8
1:4	310.0
1:3	309.7
1:2	307.8
1:1	306.0
2:1	304.2
3:1	303.9
4:1	302.6
5:1	302.7

This example shows the effect of using different ratios of iso-stearic acid and iso-stearyl alcohol.

Examples 1 and 2 use a relatively low amount of octyl triazone because of the limitations of the Lambert-Beer law.

Example 3

A sun screen formulation was made by 1) preparing separately a composition A and B, containing the ingredients listed below in the indicated amounts, by mixing the ingredients in the indicated order and heating to 75°C, 2) adding composition B slowly to composition A and mixing (400 rounds per minute), while the temperature was

maintained at 75°C and while the mixture was allowed to emulsify and 3) allowing the emulsion to cool to room temperature while gently mixing (100 rounds per minute).

Composition A	
Ingredient	Amount, % by weight
Cremophor™ A25 (emulsifier) 2)	2.50
Cremophor A6 (emulsifier) 2)	2.50
ESTOL™ 1474 (glyceryl stearate) 1)	5.00
ESTOL 3603 (caprylic, capric triglyceride) 1)	8.00
PRISORINE™ 3505 (iso-stearic acid) 1)	1.00
PRISORINE 3515 (iso-stearyl alcohol) 1)	2.00
ESTOL 1540 (octyl cocoate) 1)	6.00
PRISORINE 2021 (isopropyl isostearate) 1)	5.00
ESTOL 3609 (trioctanoin) 1)	4.00
Abil™ 100 (dimethicone) 3)	0.20
Uvinul™ M-40 (benzophenone-3/UVabsorber) 2)	3.00
Uvinul T-150 (octyl triazone) 2)	4.00

Composition B	
Ingredient	Amount, % by weight
PRICERINE™ 9091 (vegetable glycerin, humectant) 1)	3.00
Methylparaben (preservative) 4)	0.17
Propylparaben (preservative) 4)	0.03
DMDM Hydantoin (preservative) 4)	0.30
Demineralised water	53.30

- 1) supplied by Unichema International
- 2) supplied by BASF
- 5 3) supplied by Th. Goldschmidt
- 4) supplied by Jan Dekker International

The sun screen formulation is according to the present invention; in the art it would be called an 'Oil-in-water Sun screen Milk'.

It is to be noted that Composition A also is a composition according to the present

invention.

Example 4

A sun screen formulation was made as in example 3 from below compositions A and B.

Composition A	
Ingredient	Amount, % by weight
PRISORINE 3505	4.00
PRISORINE 3793 (polyglycerol-2 triisostearate) 1)	1.50
PRISORINE 3515	8.00
ESTOL 1512 (isopropyl myristate) 1)	2.00
PRISORINE 2036 (octyl isostearate) 1)	2.00
PRISORINE 2039 (isostearyl isostearate) 1)	2.00
Behenyl alcohol (stabilizer)	5.00
Abil 100	0.30
Uvinul T-150	3.00
Parsol™ 1789 (butylmethoxydibenzoylmethane, UV-absorber) 5)	2.00
PRISTERENE™ 9559 (stearic acid) 1)	4.00

Composition B	
Ingredient	Amount, % by weight
PRICERINE 9091	3.00
KOH	0.40
Methylparaben	0.17
Propylparaben	0.03
DMDM Hydantoin	0.30
Demineralised water	62.30

1) supplied by Unichema International

5 5) supplied by Givaudan-Roure

The sun screen formulation obtained was a formulation according to the present invention; in the art it would be called a 'sun lotion'. It is to be noted that composition A also is a composition according to the present invention.

CLAIMS

1. Sun screen composition, comprising octyl triazone and at least one compound selected from the group consisting of iso-stearic acid, iso-stearyl alcohol, and mixtures thereof.
- 5 2. Composition according to claim 1, characterized in that it comprises at least 0.5% by weight of octyl triazone.
3. Composition according to claim 2, characterized in that it comprises 0.5-15% by weight of octyl triazone.
4. Composition according to any of claims 1-3, characterized in that it comprises at
10 least 1% by weight of iso-stearic acid and/or iso-stearyl alcohol.
5. Composition according to claim 4, characterized in that it comprises 1-55% by weight of iso-stearic acid and/or iso-stearyl alcohol.
6. Composition according to any of claims 1-5, characterized in that it comprises iso-stearic acid and iso-stearyl alcohol in a ratio of between 1:0.5 and 1:4.
- 15 7. Composition according to any of the claims 1-6 characterized in that it further comprises ingredients conventionally used for preparing sun screen compositions including further emollients, further UV-light absorbing compounds, humectants, preservatives, emulsifiers, stabilisers, salts and water.
8. Use of a compound selected from the group consisting of iso-stearic acid and
20 iso-stearyl alcohol and mixtures thereof to cause a hypsochromic or bathochromic shift of octyl triazone in a sun screen composition.